

Light Water Reactor Sustainability Program

Initial Probabilistic Evaluation of Reactor Pressure Vessel Fracture with Grizzly and RAVEN



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Initial Probabilistic Evaluation of Reactor Pressure Vessel Fracture with Grizzly and RAVEN

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EXECUTIVE SUMMARY

The Grizzly code is being developed with the goal of creating a general tool that can be applied to study a variety of degradation mechanisms in nuclear power plant components. The first application of Grizzly has been to study fracture in embrittled reactor pressure vessels (RPVs). Grizzly can be used to model the thermal/mechanical response of an RPV under transient conditions that would be observed in a pressurized thermal shock (PTS) scenario. The global response of the vessel provides boundary conditions for local models of the material in the vicinity of a flaw. Fracture domain integrals are computed to obtain stress intensity factors, which can in turn be used to assess whether a fracture would initiate at a pre-existing flaw. These capabilities have been demonstrated previously.

A typical RPV is likely to contain a large population of pre-existing flaws introduced during the manufacturing process. This flaw population is characterized statistically through probability density functions of the flaw distributions. The use of probabilistic techniques is necessary to assess the likelihood of crack initiation during a transient event. This report documents initial work to perform probabilistic analysis of RPV fracture during a PTS event using a combination of the RAVEN risk analysis code and Grizzly. This work is limited in scope, considering only fracture initiation at a single flaw with deterministic geometry, but with uncertainty introduced in the parameters that influence fracture toughness. These results are benchmarked against equivalent models run in the FAVOR code.

When fully developed, the RAVEN/Grizzly methodology for modeling probabilistic fracture in RPVs will provide a general capability that can be used to consider a wider variety of vessel and flaw conditions that are difficult to consider with current tools. In addition, this will provide access to advanced probabilistic techniques provided by RAVEN, including adaptive sampling and parallelism, which can dramatically decrease run times.

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ACRONYMS

CPI	Conditional Probability of Initiation
MC	Monte Carlo
PTS	Pressurized Thermal Shock
PWR	Pressurized Water Reactor
ROM	Reduced Order Model
RPV	Reactor Pressure Vessel
RSM	Response Surface Methodology
SIFIC	Stress Intensity Factor Influence Coefficient

1 Introduction

The Grizzly code is being developed with the goal of creating a general tool that can be applied to study a variety of degradation mechanisms in nuclear power plant components. The first application of Grizzly has been to study fracture in embrittled reactor pressure vessels (RPVs). Grizzly can be used to model the thermal/mechanical response of an RPV under transient conditions that would be observed in a pressurized thermal shock (PTS) scenario. The global response of the vessel provides boundary conditions for local models of the material in the vicinity of a flaw. Fracture domain integrals are computed to obtain stress intensity factors, which can in turn be used to assess whether a fracture would initiate at a pre-existing flaw. These capabilities have been demonstrated previously.

A typical RPV is likely to contain a large population of pre-existing flaws introduced during the manufacturing process. This flaw population is characterized statistically through probability density functions of the flaw distributions. The use of probabilistic techniques is necessary to assess the likelihood of crack initiation during a transient event. This report documents initial work to perform probabilistic analysis of RPV fracture during a PTS event using a combination of the RAVEN risk analysis code and Grizzly.

This work has been done in close communication with the developers of FAVOR (Fracture Analysis of Vessels - Oak Ridge) [1, 2], a code specifically developed for deterministic and probabilistic analysis of reactor pressure vessels under transient conditions. FAVOR is focused solely on the beltline region of the RPV—the large unobstructed cylindrical wall of the RPV directly in-line with the reactor core. That region experiences the highest level of irradiation and is thus the region most sensitive to embrittlement, making it particularly susceptible to failure by fracture. Grizzly results, both deterministic and probabilistic, have been benchmarked against FAVOR results in this report.

Ultimately, a probabilistic fracture mechanics analysis of an RPV must consider the combined effects of a large population of flaws with uncertain properties. This report documents initial work toward the goal of such an analysis. To simplify the procedure for this initial step, only crack initiation at a single flaw with prescribed geometry is considered. Uncertainty is included in the properties that affect the embrittlement and fracture capacity of the material. To incorporate uncertainty in the flaw geometry, it is necessary to have simplified representations of fracture models that can be rapidly evaluated. Progress has been made toward developing reduced order models to efficiently compute fracture parameters in Grizzly, and is documented here, but more work remains to integrate these models into the tools used here for probabilistic fracture mechanics analysis.

This report is organized as follows: Section 2 summarizes the steps required to perform a deterministic fracture analysis of a single flaw in an RPV, provides a demonstration of such an analysis in Grizzly, and compares those results with those from an equivalent FAVOR simulation. Section 3 describes the RAVEN probabilistic framework and its integration with Grizzly, demonstrates RAVEN/Grizzly probabilistic fracture mechanics simulation results for a single flaw, and compares those results with a RAVEN/FAVOR and a FAVOR simulation. Section 4 shows the progress of work underway to develop reduced order models of fracture based on Grizzly models, and the procedure for integration of these with RAVEN. Finally, Section 5 summarizes this work and plans for future development in this area.

2 Deterministic Fracture Analysis

A capability for deterministic analysis of fracture initiation at flaws of defined geometry under pressurized thermal shock conditions is a necessary foundation for a probabilistic fracture mechanics analysis of an RPV. Prior reports [3, 4] have documented the development and application of domain integral techniques for evaluation of fracture parameters in Grizzly.

A deterministic assessment of crack initiation in an RPV under transient consists of three major components:

- **Global Thermo-Mechanical Response** The global thermo-mechanical response of the RPV under a transient loading history is computed without considering the effects of flaws. Prior reports demonstrated Grizzly simulations of 3D RPVs. This is the most general case, and permits the evaluation of effects that cannot be represented with lower dimensionality models, such as effects due to nonuniformities in the thermal state and geometric nonuniformities, such as those that occur in the nozzle regions. Most RPV fracture analyses focus on the beltline region because the highest neutron fluence and highest embrittlement occur there, and a 2D or 1D representation is sufficient to capture the global RPV response in that region. Grizzly now has the capability, which is used in the current application, to represent the global response using a single row of elements and appropriate boundary conditions and constraints in 2D for more efficient analyses in that case.
- **Stress Intensity Factors** Linear elastic fracture mechanics is used to assess brittle fracture in RPVs under transient conditions. Flaws aligned in the axial or circumferential directions are subjected to pure Mode-*I* loading. The Mode-*I* stress intensity factor, K_I is computed as a function of time at locations along the 3D crack front and used as a measure of the loading applied to the crack. This is currently done using a detailed 3D finite element model of the material in the vicinity of the crack tip that includes the crack geometry, and which has prescribed boundary conditions derived from the response history of the global 2D or 3D RPV model. The detailed 3D fracture model is computationally expensive, which is not a serious problem for the current study, where a single flaw is evaluated. It would, however, be impractical for use in a probabilistic fracture mechanics analysis in which a large number of flaw geometries are considered. For that reason, a procedure to construct and use a reduced order model (ROM) to efficiently compute fracture parameters with Grizzly and RAVEN is being developed, and is summarized in Section 4. This will be applied in future probabilistic analyses of realistic flaw populations.
- **Initiation** Once the loading on a flaw has been characterized, the final step is to assess whether the loading exceeds the capacity of the flaw to resist fracture, resulting in the initiation of a crack at that flaw. This consists of evaluating the extent of embrittlement at the flaw location, which is characterized as a shift in the nil-ductility temperature, ΔRT_{NDT} , and evaluating the toughness at the current temperature. Multiple models have been developed for computing the transition temperature shift due to embrittlement. The model employed here is that of [5], and is one of the options provided by FA-VOR. At a given embrittlement level and temperature, there is significant statistical variation in the fracture toughness, K_{IC} , which is characterized with a Weibull distribution. Because of this, the most “deterministic” result that can be computed from the analysis of a single flaw with deterministic geometry and loading conditions and material properties is the time history of the instantaneous conditional probability of initiation (CPI) computed from the Weibull distribution. The maximum value of that instantaneous CPI during a transient event is the quantity computed from each random realization in a probabilistic fracture analysis.

Pre-existing capabilities in Grizzly to compute stress intensity factors on 3D fracture models were combined with new capabilities for efficient evaluation of the response of the beltline region of an RPV with a

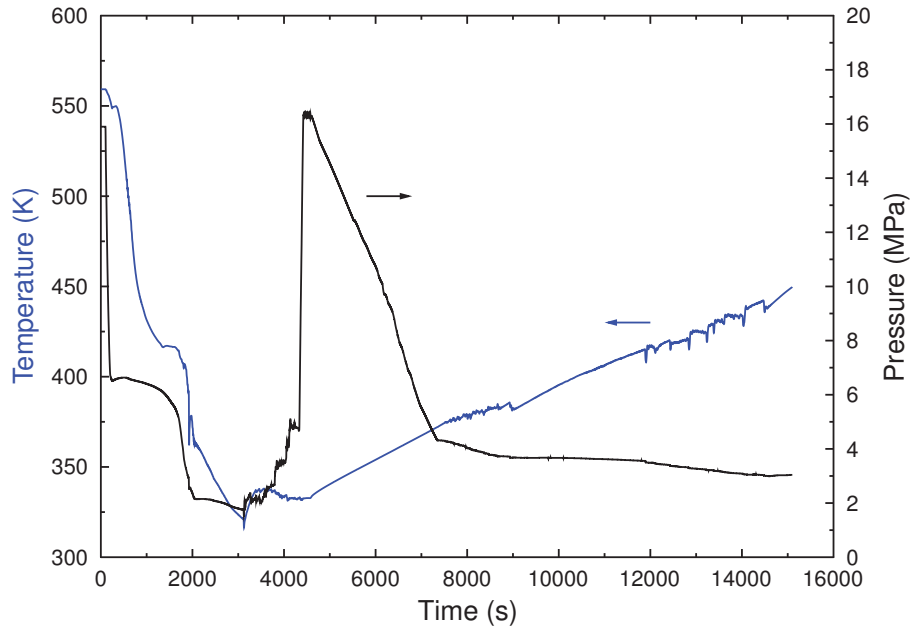


Figure 1: Time histories of coolant temperature and pressure applied as boundary conditions to global RPV model.

2D model. In addition, a Python code module was developed to plug in to RAVEN to read the time history of the stress intensity and temperature from a Grizzly model, compute the embrittlement as a function of uncertain parameters, and compute the maximum CPI for a given random realization of a flaw.

To benchmark the deterministic fracture models developed in Grizzly, a special modified version of the FAVOR probabilistic fracture mechanics module (FAVPFM) that performs a deterministic analysis of a single flaw with a prescribed set of parameters relating to the steel chemical composition was developed. This module, known as FAVDFM (for FAVOR Deterministic Fracture Mechanics), reads the global thermo-mechanical beltline response from a prior FAVLOAD run, computes the stress intensity factor and temperature history, and computes the maximum CPI, permitting a direct comparison. This module was used to benchmark a deterministic Grizzly simulation. In addition, as is documented in later sections of this report, it was driven by RAVEN to perform a probabilistic fracture mechanics analysis of a single flaw with uncertain parameters affecting the fracture capacity for benchmarking of the RAVEN/FAVDFM model against equivalent RAVEN/Grizzly and FAVPFM models.

2.1 Deterministic Grizzly models

A representative geometry for a pressurized water reactor (PWR) RPV was used for all of the models presented here. The inner radius is 86.5 in, the overall thickness with the cladding is 8.65 in, and the cladding thickness is 0.156 in. This model was subjected to a transient event in which the coolant temperature and pressure follow the histories shown in Figure 1, which is a particularly severe transient with a low probability of occurrence. Figure 2 shows the 2D finite element model used to represent a strip of the material in the beltline region. Quadratic, 8-noded quadrilateral elements are used with an axisymmetric formulation.

The coolant pressure is applied to the inner (leftmost) boundary, and a convective flux thermal boundary condition with a time-varying heat transfer coefficient to the inner boundary. The bottom nodes are fixed



Figure 2: Finite element mesh used in 2D strip model of RPV beltline region. The two elements on the left hand side with lighter shading represent the stainless steel liner, and the remaining, darker shaded elements on the right are for the base metal.

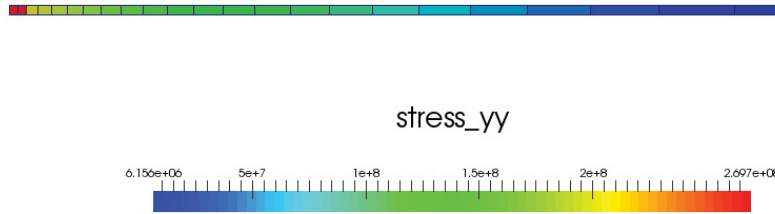


Figure 3: Stress field (axial direction) computed by strip model at a time 4800s from start of transient. Individual elements are colored by the element average values.

against displacement in the vertical direction, and a constraint is applied to the displacement degrees of freedom on the top surface in the vertical direction to permit free movement as a group, but restrict them to all have the same value. This treats the body as an infinite cylinder, forcing planar sections to remain planar, but permitting axial strains due to thermal expansion and pressure loads. Figure 3 shows a representative contour plot of the axial stress field in this model at a time 4800s into the transient, when a spike in the pressure has occurred. This model requires significantly less computational resources than a detailed 3D model, but accurately captures the response of the beltline region in cases when there are no features to cause local irregularities in the stress field.

Figure 4 shows the 3D finite element model used to represent an axially-oriented surface-breaking flaw in Grizzly. The aspect ratio (flaw width/depth) of this flaw is 6. This model includes the base metal and liner. Two orthogonal symmetry planes pass through the flaw. A recently developed MOOSE function called `Axisymmetric2D3DSolutionFunction` is used to read solution fields from a 2D axisymmetric model and transform them to equivalent fields in a 3D model. These fields, which are interpolated in time and space, are applied as Dirichlet boundary conditions to the displacement fields on the outer boundaries of this model, and to directly compute the temperature solution everywhere in this model.

Figure 5 shows a comparison of the time histories of the Mode- I stress intensity K_I computed by Grizzly and FAVOR during the transient event. Figure 6 shows a similar comparison of the temperature histories at the flaw tips computed by the two codes. While the computed temperatures are nearly identical, the Grizzly-computed stress intensity factor is roughly 5% lower than that computed by FAVOR. One source of the difference between the two results is that the FAVOR result includes the effect of pressure applied to the crack face, while the Grizzly result does not. FAVOR has an option to not include this contribution, and the FAVOR result without that contribution is also shown in Figure 6, and is closer to the Grizzly solution. A preliminary capability to compute that contribution has been developed in Grizzly, and will be ready for use in the near future. The remaining discrepancies between the two codes will also be addressed.

Once the time histories of K_I and temperature are computed, they can be used to compute the maximum CPI for that transient. An embrittlement model has been used to compute a transition temperature shift, which is done once per flaw realization. This is done internally in FAVDFM, and is computed by the RAVEN plugin

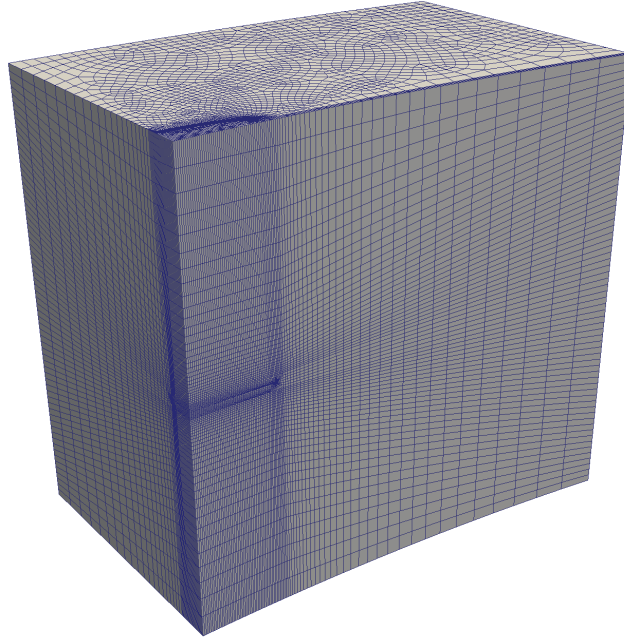


Figure 4: 3D Finite element model of circumferential flaw penetrating 1/10 through the wall thickness, and with a ratio of flaw width to depth of 6.

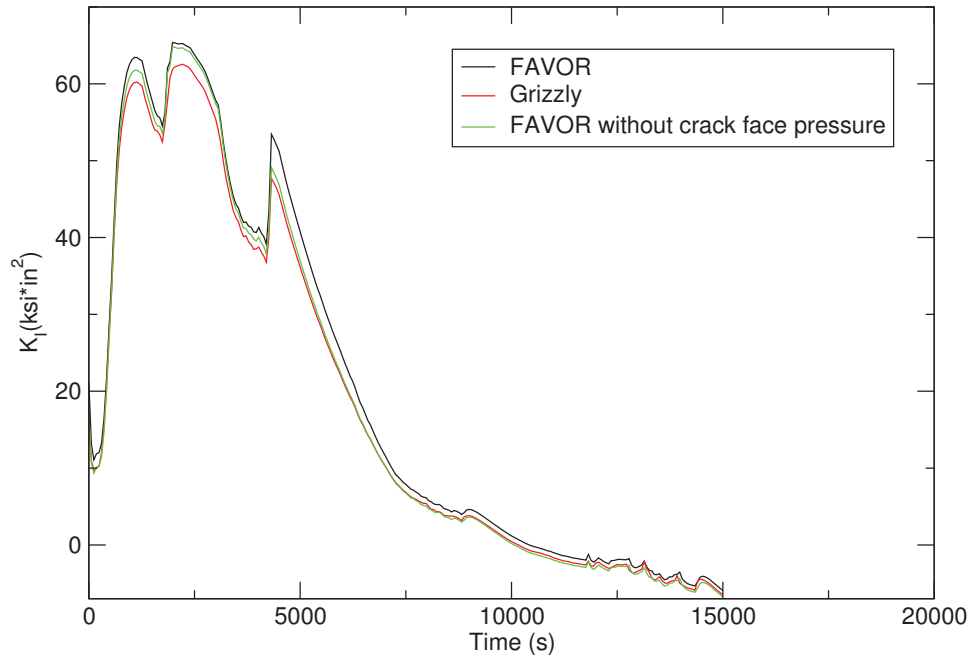


Figure 5: Time history of K_I computed by Grizzly and FAVOR. FAVOR results are also shown without considering the crack face pressure, which was not considered in the Grizzly analysis.

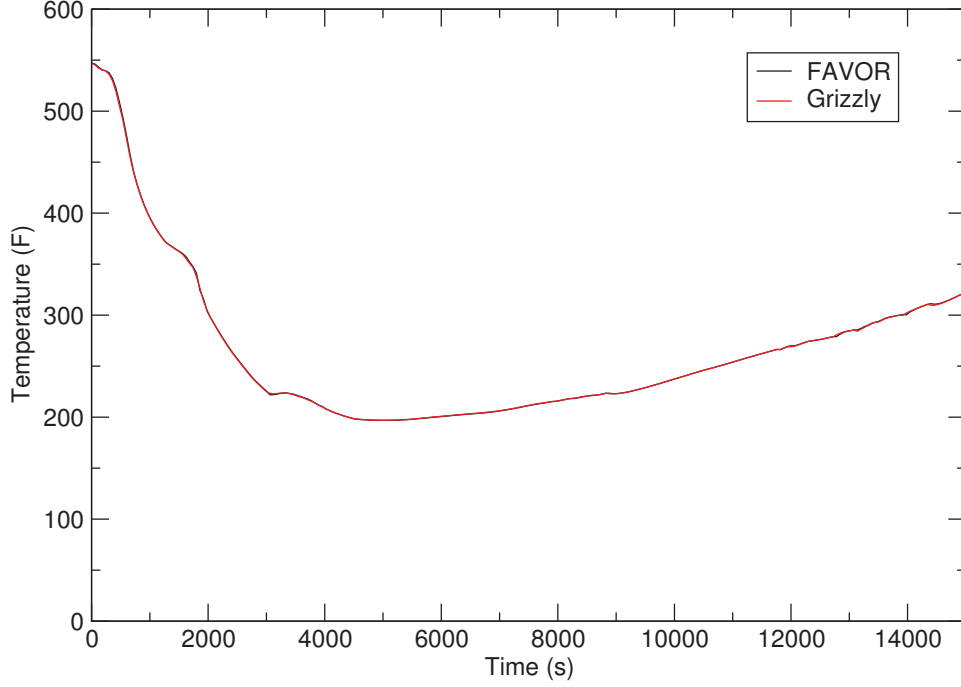


Figure 6: Time history of temperature computed by Grizzly and FAVOR.

Table 1: Parameters used to compute deterministic embrittlement and CPI in FAVOR and Grizzly

Parameter	Value
Effective full power years	40
Surface fluence (n/cm ²)	2e+19
Cu (Weight %)	0.213
Ni (Weight %)	1.010
Mn (Weight %)	1.315
P (Weight %)	0.019
Initial RT_{NDT} (F)	0.0

for Grizzly. The parameters used for the computations in both of these codes are shown in Table 1.

Equations 1-4, are used to compute the parameters for the temperature-dependent Weibull distribution and the instantaneous conditional probability of initiation in FAVOR, and have been implemented in the Grizzly RAVEN plugin. In these equations, ΔT_{rel} is the difference between the current temperature, T , and the nil-ductility temperature ($\Delta T_{rel} = T - RT_{NDT}$). Figure 7 shows a contour plot of CPI as computed with this temperature-dependent Weibull distribution. The black line in this plot is the $a_{K_{IC}}$ parameter in the Weibull distribution, and represents the lower bound value of K_I for which CPI is nonzero. In the region below that line (shown in white), CPI is zero. Figure 8 shows the time history of CPI computed by the Grizzly RAVEN plugin, with a comparison with the FAVOR results. The instantaneous CPI was computed by the Grizzly RAVEN plugin in two ways: using the Grizzly-computed K_I history and using the FAVOR-computed K_I history. The CPI history computed by the Grizzly plugin is nearly identical to that computed by FAVOR when the FAVOR K_I history is used, and as would be expected, it is somewhat lower when the Grizzly K_I history is used because the stress intensity is somewhat lower in that case. This gives confidence

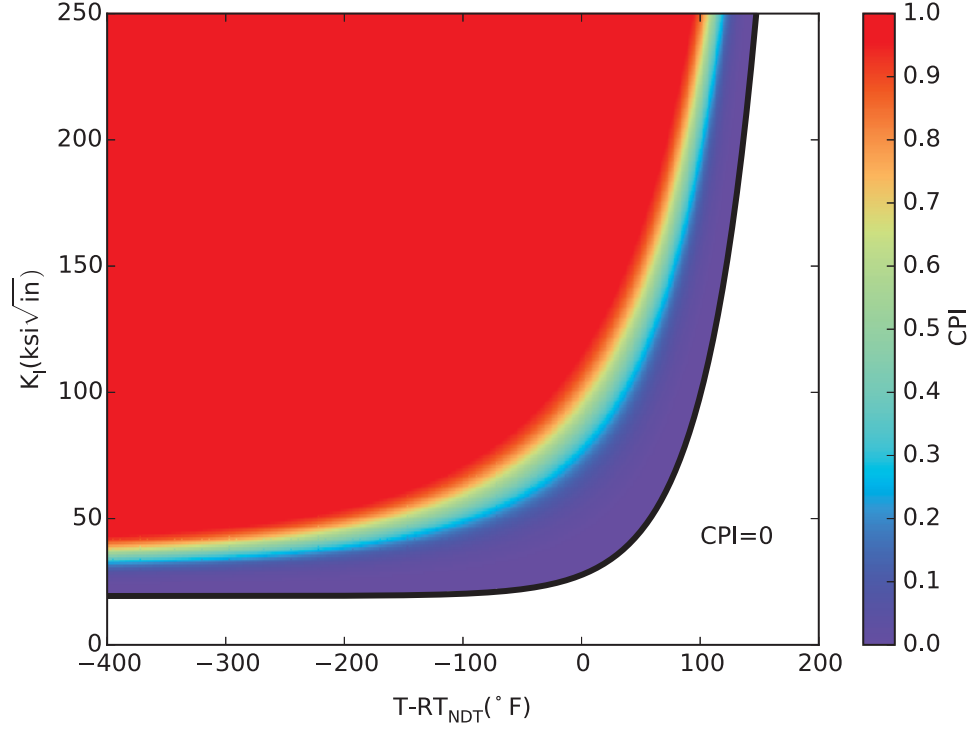


Figure 7: Conditional probability of initiation (CPI) as a function of temperature and K_I

in the procedure for computing CPI with the Grizzly RAVEN plugin.

$$a_{K_{IC}}(\Delta T_{rel}) = 19.35 + 8.335 \exp(0.02254 * \Delta T_{rel})(\text{ksi}\sqrt{\text{in}}) \quad (1)$$

$$b_{K_{IC}}(\Delta T_{rel}) = 15.61 + 50.132 \exp(0.008 * \Delta T_{rel})(\text{ksi}\sqrt{\text{in}}) \quad (2)$$

$$c_{K_{IC}} = 4.0 \quad (3)$$

$$\text{CPI}(\Delta T_{rel}, K_I) = \begin{cases} 0 & \text{if } K_I < a_{K_{IC}} \\ 1 - \exp\left(-\left[\frac{K_I - a_{K_{IC}}}{b_{K_{IC}}}\right]^{c_{K_{IC}}}\right) & \text{otherwise} \end{cases} \quad (4)$$

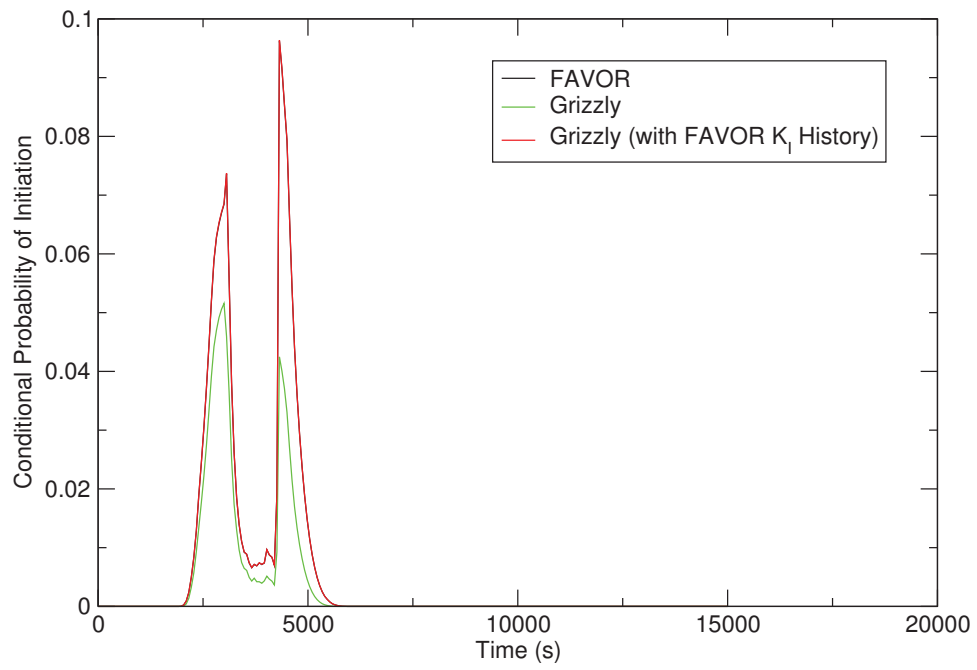


Figure 8: Time history of instantaneous conditional probability of initiation from Grizzly and FAVOR models. The Grizzly model was also run using the FAVOR K_I history for comparison.

3 Probabilistic Fracture Analysis of Single Flaw

The next step of this effort was to perform probabilistic analyses of the susceptibility of a single flaw to fracture with uncertain material properties. These analyses were performed using a combination of the RAVEN probabilistic framework, Grizzly, and components of the FAVOR tools. The following analyses were performed:

- **RAVEN/Grizzly:** RAVEN was used for Monte Carlo sampling of Grizzly and the RAVEN plugin described in the previous section to compute the maximum CPI under a given transient with given material properties.
- **RAVEN/FAVDPM:** RAVEN was used to drive the special deterministic version of FAVOR, FAVDFM, that was developed specifically for benchmarking Grizzly calculations.
- **FAVPFM:** The probabilistic module of FAVOR, FAVPFM, was used to perform a probabilistic analysis of a single flaw with uncertain material properties.

In this section, an overview of RAVEN is provided, followed by a summary of the probabilistic analyses performed in these three ways.

3.1 RAVEN overview

RAVEN was developed in a highly modular and pluggable way to enable easy integration of different programming languages (i.e., C++ and Python) and coupling with any system/physics code. Its main goal is to provide a tool to allow exploration of the uncertain domain, dispatching several different capabilities in an integrated environment.

The main idea behind the design of the RAVEN software package is the creation of a multi-purpose framework characterized by high flexibility with respect to the possible set of analyses that a user might request. To obtain this result, the code infrastructure must be capable of constructing the analysis/calculation flow at run-time, interpreting the user-defined instructions, and assembling the different analysis tasks following a user-specified scheme.

The need to achieve such flexibility, combined with reasonably fast development, pushed toward the programming language that is naturally suitable for this kind of approach: Python.

Hence, RAVEN is coded in Python and characterized by a highly object-oriented design. The core of the analysis available through RAVEN is represented by a set of basic components (entities) the user can combine, to create a custom analysis flow. A list of these components and summary of their most important functionalities are as follows:

- **Distribution:** The probability of a specific system outcome is related to the probability of the set of input parameters and initial conditions that led to such an outcome. Moreover, some sampling techniques (e.g., Monte-Carlo [MC]) explore the input space according to the probabilistic distribution associated to the input variables. Consequently, RAVEN possesses a large library of PDFs.
- **Sampler:** A proper approach to sample the input space is fundamental for optimizing the computational time. In RAVEN, a “sampler” determines a unique exploration strategy that is applied to the input space of a system. The association of uncertain variables and their corresponding probability distributions constitute the probabilistic input space on which the sampler operates.
- **Model:** A model is the representation of a physical system (e.g., a nuclear power plant); it is therefore capable of predicting the evolution of a system given a coordinate set in the input space (i.e., the initial

condition of the system phase space). A model usually, does not belong to RAVEN but it is made available to RAVEN by the user either by the available APIs or by coding it directly inside RAVEN as external model.

- **Reduced Order Model:** The evaluation of the system response, as a function of the coordinates in the uncertain domain (also known as input space), is very computationally expensive, which makes brute-force approaches (e.g., MC methods) impractical. Reduced order models (ROMs) are used to lower this cost by reducing the number of needed points and prioritizing the area of the uncertain domain that needs to be explored. They are a pure mathematical representation of the link between the input and output spaces for a particular system.
- **Post-Processors:** The post-processors are used to process the datasets resulting from a simulation of a system either in RAVEN or via an external code. Post-processors can be used to obtain basic statistical information of the data, compare datasets statistically, or discover patterns in the datasets, i.e. data mining. The list above is not comprehensive of all the RAVEN framework components, which also include visualization and storage infrastructure.

3.2 RAVEN/Grizzly

The module to compute the embrittlement and the time history of CPI as a function of K_I and temperature that was mentioned in the previous section was developed in Python and integrated in RAVEN using what is known in RAVEN as an `ExternalModel`. Prior to the RAVEN run, a single deterministic analysis of the global RPV response and a fracture mechanics analysis of the 3D flaw region model were performed, as described in Section 2. A RAVEN model was set up to perform Monte Carlo sampling of the parameters listed in Table 2, and run the RAVEN/Grizzly `ExternalModel` to compute the maximum CPI for each realization.

Table 2: Parameters for normal distributions of uncertain parameters in RAVEN/Grizzly probabilistic analysis

Parameter	Mean	Standard Deviation
Surface fluence (n/cm ²)	2e+19	0.19234e19
Cu (Weight %)	0.213	0.0073
Ni (Weight %)	1.010	0.0244
Mn (Weight %)	1.315	0.05
P (Weight %)	0.019	0.0013
Initial RT_{NDT} (F)	0.0	17.0

These random distributions are for the most part equivalent to what is used by FAVPFM. One important discrepancy between the two is that for the distribution of the Mn content, FAVPFM uses a normal distribution for the Mn content of the first flaw in a plate, with a variance that is computed separately for each plate using a Weibull distribution. To simplify the analysis here, a single value was used for the variance for the Mn distribution.

Each evaluation of the `ExternalModel` is very rapid, and the sampling was performed in parallel. Using 4 cores on a workstation, 10000 samples were evaluated in less than 30 seconds.

Because of the discrepancies in the K_I history computed by FAVOR and Grizzly mentioned in Section 2, the RAVEN/Grizzly probabilistic analysis procedure was run two times: once using the Grizzly-computed K_I history, and once using the FAVOR-computed K_I history. It is expected that the results produced using the FAVOR K_I history should match well with probabilistic results from FAVOR, while results produced

using the Grizzly K_I history should give lower values for CPI. Using the Grizzly-computed K_I history, the mean value of the CPI is 0.0703, while using the RAVEN-computed K_I history, the mean value of CPI is 0.1179.

While only the mean values of CPI are reported here, it should be mentioned that RAVEN provides extensive capabilities to visualize results and to report a variety of statistics on the distribution of the output variables and the sensitivity of the target quantities to the uncertain parameters in the input space.

3.3 RAVEN/FAVDPM

An interface to call FAVDPM from RAVEN to compute CPI for a single flaw was developed for benchmarking purposes. A special model based on RAVEN's `GenericInterface`, known as `FAVORInterface` was developed for this purpose. This interface, written in Python, runs FAVDPM for a given realization and parses the output to obtain the values for RT_{NDT} and CPI, which are then returned to RAVEN.

Using 10000 samples, the mean CPI computed from this RAVEN/FAVDPM analysis was 0.1068.

3.4 FAVPFM

Finally, the FAVOR probabilistic tool, FAVPFM, was used to perform an equivalent probabilistic analysis of a single flaw using the same parameters as used for the other cases. FAVPFM is typically used to evaluate large populations of flaws distributed through the various regions of an RPV. Parameters were adjusted in the standard FAVPFM input files to force it to evaluate a single flaw for comparison with the other approaches evaluated here. The mean CPI computed after 10000 Monte Carlo samples with FAVPFM was 0.1007.

3.5 Discussion

It has been demonstrated that the RAVEN/Grizzly model for a single crack gives reasonable agreement with FAVOR, run both in a mode where FAVOR was sampled by RAVEN, and with FAVOR doing the sampling internally. The main discrepancies in the results are due to the differences in the time histories of K_I computed by Grizzly and FAVOR, which are being investigated. There are other differences in the sampling procedures used by FAVPFM and RAVEN/Grizzly that are likely also contributing to the difference in the results, and these will be the subject of future investigation.

The current study has been limited to studying crack initiation in a single flaw. Much more work is still required to perform a probabilistic analysis of a realistic flaw population. A major necessary component of that is the ability to rapidly evaluate the stress intensity for a single flaw realization. In addition, it is important to note that the current study only considers crack initiation. The probability of failure due to crack propagation through the wall of the RPV is also an important quantity of interest computed by FAVOR.

4 Reduced Order Models for Fracture

As mentioned previously, to evaluate a realistic flaw population in a full RPV simulation, it is critical to have a technique for rapid computation of the time history of the stress intensity, which is computed using a computationally expensive 3D model in the current work in Grizzly. Work is underway to develop a procedure to compute this using a reduced order model, which can be evaluated within the module developed for evaluation of CPI in RAVEN.

The approach taken here is to use the procedure that has been used successfully in FAVOR to rapidly evaluate K_I for axis-aligned flaws, but within the framework of a response surface. Once this has been successfully demonstrated, this procedure can be extended to automatically generate models that can represent a wider variety of flaw geometries, such as off-axis flaws.

4.1 Influence Coefficient Methodology

For surface-breaking flaws, FAVOR utilizes a database of stress intensity factor influence coefficients (SIFICs) developed at Oak Ridge National Laboratory and a weighting-function approach to calculate the stress intensity at locations along the tip of a flaw throughout the transient. The database of SIFICs was created using 3D finite element models run in another code (Abaqus) for a range of crack aspect ratios ($L/a = 2, 6, 10$), relative crack thicknesses ($.01 < (a/t) < .5$) and angular positions along the crack front ($\phi = 0 - 90$). As pointed out in the FAVOR theory manual, the study in [6] indicates that there is very little difference between the SIFICs for axial and circumferential flaws with a relative depth of $(a/t) < .5$. For the cladding, SIFICs are also tabulated with an additional parameter, the cladding's thickness, for thicknesses of 0.156 and 0.25 inches.

FAVOR's deterministic capability provides a useful measure for benchmarking results obtained from Grizzly. For a purely deterministic analysis of a surface breaking flaw, FAVOR runs a one-dimensional finite element analysis on the un-cracked structure for the given material properties, RPV geometry and thermo-mechanical boundary conditions. The stress intensity factors for mode- I loading (axial and circumferential flaws in this case) with the presence of cladding are obtained using the following equation:

$$K_I = K_{Ib} + K_{Icl} \quad (5)$$

where K_{Ib} and K_{Icl} are the contributions to K_I from the base metal and cladding, respectively.

The total stress intensity factor solution is found by first calculating the stress intensity for the base material, then the stress intensity for the cladding. Each K_I solution is found by superimposing the stress intensity due to the terms in a third-order polynomial expansion of the stress field from the inner wetted surface of the vessel to the crack tip:

$$K_I = \sum_{j=0}^3 C_j \sqrt{\pi a} K_j \quad (6)$$

where a is the crack depth and C_j are the terms in the following polynomial expansion of the stress field:

$$\sigma(a') = C_0 + C_1 \left(\frac{a'}{a} \right) + C_2 \left(\frac{a'}{a} \right)^2 + C_3 \left(\frac{a'}{a} \right)^3 \quad (7)$$

in which a' is the distance from the inner wetted surface. K_j are the SIFICs, which are tabulated in the FAVOR theory manual[2].

The same equation is used for both the cladding and base material, however, only the constant and linear terms in the polynomial are used for the cladding. The values and quantities of the K and C coefficients

thus differ for the base and cladding materials. For the base material, K_{Ib} , j is indexed from 0 to 3. C_j are the coefficients obtained by fitting a cubic polynomial to the stress in the un-cracked structure over the total length of the given flaw. This is done using a least squares polynomial fit, which represents the stress as a function of the radial distance measured from the interface of the base and cladding material over the normalized crack length.

For the effect of the stress in the cladding on K_I , j is indexed from 0 to 1. The K_j are tabulated stress intensity influence coefficient (SIFIC) values for the cladding, which differ from the base metal K_j values as they are also a function of clad thickness. To compute the C coefficients that describe the stress field in the cladding, two lines are created through the thickness of the cladding. The first, σ_{clad} , is the measured stress using two nodes in the cladding. The second, σ_{total} is a linear extrapolation through the cladding using the stress in the first two nodes of the base metal. The required C coefficients are then found by computing $(\sigma_{total} - \sigma_{clad})$.

Currently, for deterministic analyses of surface breaking flaws, FAVOR can consider only aspect ratios of 2, 6, 10, and infinity. Also, although the SIFICs are parameterized with respect to angular position along the crack front, FAVOR only considers the deepest position on a surface-breaking flaw. Therefore, the only parameters describing the crack geometry used by FAVOR for considering an individual surface-breaking flaw are the crack depth and cladding thickness. To obtain SIFIC values for general a/t ratios and cladding thicknesses, FAVOR uses an interpolation scheme.

4.2 Influence Coefficient Methodology in Grizzly

A technique to use the influence coefficient methodology described in the previous section is being developed for use in the framework of RAVEN/Grizzly. RAVEN provides capabilities for performing sampling of a detailed physics model within an input parameter space, and using that data as input to a variety of types of reduced order model (ROM). This can be a powerful technique for automatically generating models that can provide K_I for a wide variety of flaw geometries.

The first step in developing this capability to evaluate more general flaw geometries is to first generate a ROM to represent the axis-aligned flaw geometries for which FAVOR already interpolates tabulated solutions to generate confidence in this methodology. As a first step, a ROM has been developed using the tabulated SIFIC data employed by FAVOR. The next step is to use RAVEN to perform grid sampling of Grizzly fracture models to automatically generate similar data. Once this has been demonstrated to give accurate results for the flaw geometries currently considered by FAVOR, this methodology will be extended to other geometries.

Progress in development of this methodology and the procedure employed to implement it in RAVEN and Grizzly are described below.

4.2.1 Least squares fit of stress

The first step in the process of using a reduced order model to compute stress intensity factors in Grizzly is to represent the response of the global RPV model with a limited number of parameters. The SIFIC methodology employed by FAVOR is employed here. Least squares fitting is performed on the through-wall stress profile in the global RPV model to obtain the coefficients in Equation 7.

A code module has been developed in MOOSE/Grizzly to extract stresses along a row of elements intersected by an arbitrary line, and to optionally perform least squares fitting on those stresses. This can be done on 2D or 3D global models of the RPV. In the work shown here, a 2D model similar to that shown in Figure 2 was used.

For a cubic least squares regression, four data points are required. However, additional points would ensure a more accurate fit. Therefore, the model requires a mesh such that the crack length spans a minimum of four integration points in the base material as well as two integration points in the cladding.

4.2.2 Response surface using FAVOR data to compute K_I

To compute K_I from the stress profile using Equation 6 requires SIFICs K_j for the flaw geometry under consideration. The FAVOR theory and Implementation manual [2] includes a large database of these values, each corresponding to a particular flaw and RPV geometry. To evaluate different flaw depths, FAVOR interpolates between those values. One alternative to interpolation between data is the utilization of least squares response surface methodology (RSM). RSM provides robust representation of the data as a closed form equation.

To test the applicability of RSM for computing the SIFICs, this technique was first applied using the tabulated data in the FAVOR theory manual. Using RSM, the SIFICs can be found as a function of all of the predictor variables (crack and RPV geometry). RSM does not require any of the flaw parameters to be values that correspond exactly to the data, allowing for any value within the range of expected parameters.

By changing the method of obtaining the correct SIFICs from interpolation between data to the evaluation of a response surface, it is possible to obtain the K_I solution for any of the parameters previously mentioned at no significant reduction in accuracy. The resulting SIFICs from a response surface will differ slightly from the interpolated values FAVOR obtains. However, interpolation may not always fully capture the trend of the data, specifically the interaction between two or more predictor variables.

4.3 Demonstration of response surface method using FAVOR data

To demonstrate the response surface methodology using data from FAVOR, both FAVOR and Grizzly were used to simulate the same PTS event, which is the same one used in the analyses in Section 2. Both models were evaluated using the same RPV dimensions and temperature-dependent material properties. Figures 9, 10, and 11 show comparisons of the time history of K_I computed using the SIFIC computed three ways: using FAVOR, using Grizzly with the response surface (with the FAVOR tabulated SIFIC data), and using Grizzly with that same SIFIC data, but linearly interpolating between the tabulated data. These figures show results for a flaw with three different aspect ratios.

As can be seen from these figures, the results for all three cases are very similar. In the cases where they differ, the Grizzly results with interpolation more closely match the FAVOR results, as would be expected since FAVOR also employs a similar interpolation scheme. The very similar results also demonstrate that Grizzly's computed global RPV response is almost identical to that obtained from FAVOR.

4.3.1 Automatic generation of data for reduced order model

Now that confidence has been developed that the RSM methodology can be successfully used to compute K_I for a variety of flaw geometries using the tabulated FAVOR data, the next step is to develop a procedure to use RAVEN to perform sampling on a Grizzly fracture model to automatically generate similar data and store it for use in a ROM for efficient probabilistic fracture mechanics analysis of RPVs.

The development of this procedure is well underway. Because the parameters being sampled affect the flaw geometry, a new computational mesh must be generated for each sample. RAVEN provides an interface to sample using the Cubit mesh generation code and MOOSE to generate a new mesh for each sampled analysis. A parameterized meshing script has been developed to automatically generate fracture meshes with Cubit for arbitrary flaw dimensions. Once this procedure is fully developed, it is expected to enable automated, rapid development of a general ROM to represent a variety of flaw geometries.

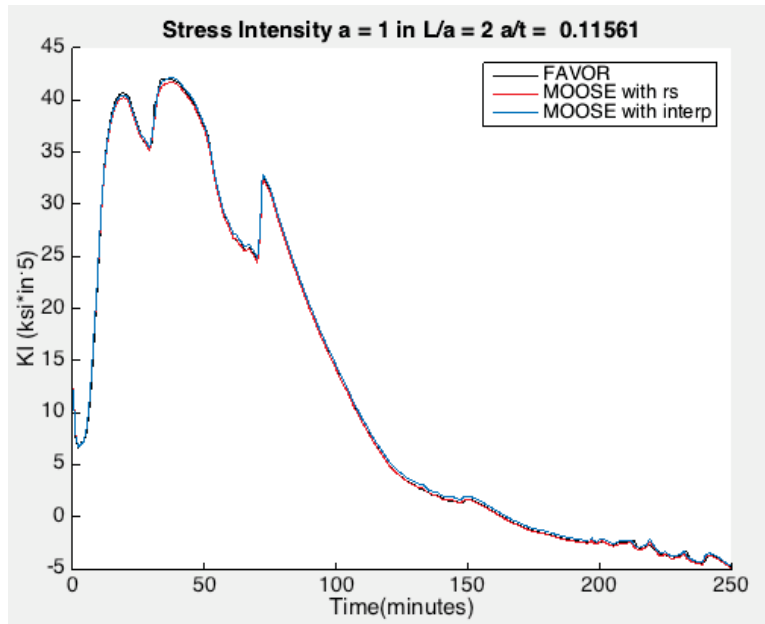


Figure 9: Time history of K_I for a flaw with an aspect ratio of 2 computed with influence coefficients three different ways: with FAVOR, with Grizzly using a response surface for the SIFICs, and with Grizzly using interpolated values for the SIFICs

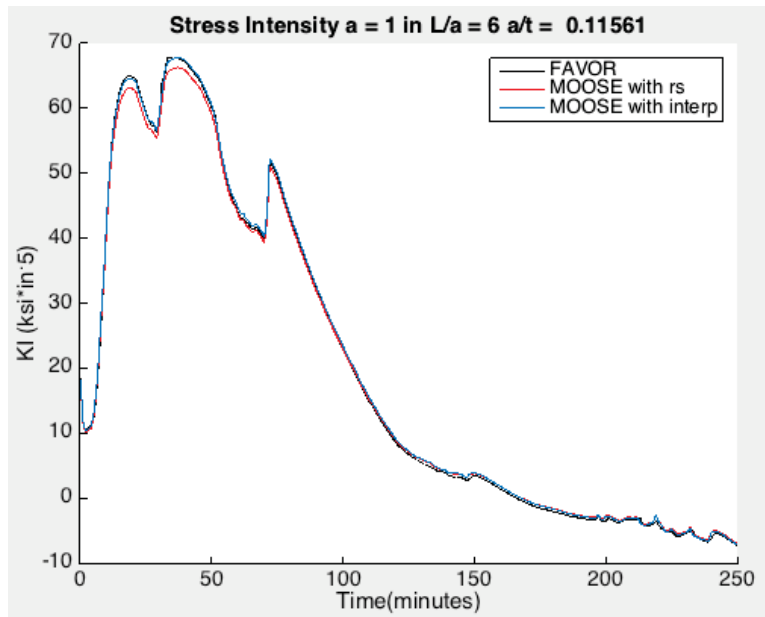


Figure 10: Time history of K_I for a flaw with an aspect ratio of 6 computed with influence coefficients three different ways: with FAVOR, with Grizzly using a response surface for the SIFICs, and with Grizzly using interpolated values for the SIFICs

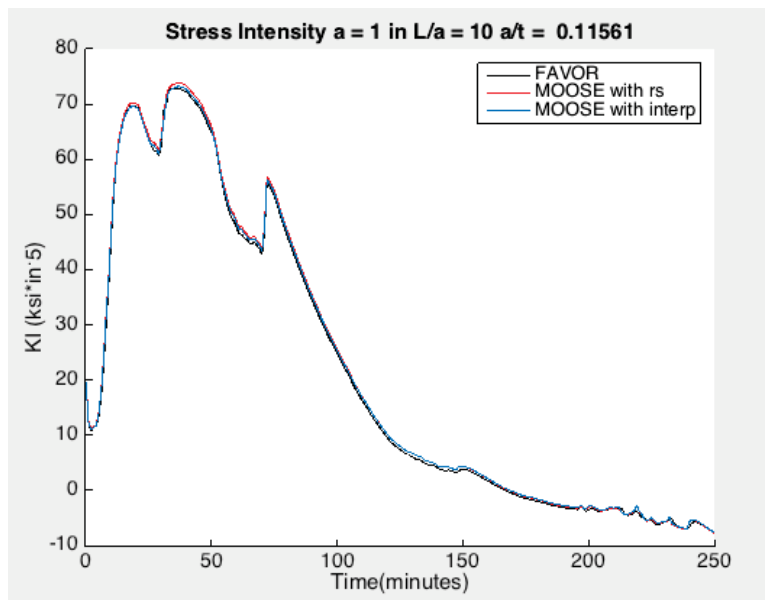


Figure 11: Time history of K_I for a flaw with an aspect ratio of 10 computed with influence coefficients three different ways: with FAVOR, with Grizzly using a response surface for the SIFICs, and with Grizzly using interpolated values for the SIFICs

5 Summary and Future Development

This report documents initial steps to perform a probabilistic fracture mechanics analysis of crack initiation in an idealized reactor pressure vessel under a pressurized thermal shock transient event using the RAVEN probabilistic framework and the Grizzly component aging simulation code. This initial analysis is limited in scope, considering crack initiation at a single flaw with deterministic geometric properties. Uncertainty was introduced in the parameters affecting material embrittlement.

In support of this initial analysis, the following code developments were made:

- A module was developed for RAVEN to compute the embrittlement and conditional probability of initiation of a flaw given time histories of stress intensity and temperature provided by Grizzly.
- A special deterministic version of FAVOR was developed for the purpose of benchmarking deterministic and probabilistic Grizzly models.
- An module was developed for RAVEN to call the special deterministic version of FAVOR to compare the probabilistic methods used by FAVOR and RAVEN.

In addition, significant progress has been made toward developing a general reduced order model capability that will be generated by RAVEN driving a Grizzly model, and used within a RAVEN probabilistic simulation to efficiently represent the fracture response of arbitrary flaws. Work will continue to complete this reduced order model capability and apply it to probabilistic analysis of general flaw populations.

When complete, the RAVEN/Grizzly approach being developed will provide the following benefits for probabilistic fracture analysis of RPVs under transient conditions:

- Grizzly and RAVEN are both built on modern, flexible code infrastructures that provide many basic facilities that are leveraged for this specific application.
- RAVEN provides advanced techniques that can greatly speed up the process of probabilistic fracture analysis, including adaptive sampling techniques and parallel processing.
- The 2D and 3D capabilities provided by Grizzly can be used to represent local nonuniformities in the global reactor pressure vessel response, such as local geometric effects and effects introduced by a nonuniform thermal environment.
- The reduced order model capability being developed in Grizzly will permit automated generation of models that can be rapidly evaluated for a wide variety of flaw configurations.

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